ON EVOLUTION EQUATIONS OF QUANTUM-CLASSICAL SYSTEMS

V.I. Gerasimenko*

Institute of Mathematics NASU,

3, Tereshchenkivs'ka str.,

01601 Kyiv, Ukraine

Abstract

We consider the links between consistent and approximate descriptions of the quantum-classical systems, i.e. systems are composed of two interacting subsystems, one of which behaves almost classically while the other requires a quantum description.

PACS numbers: 03.65.-w, 03.65.Sq, 05.30.-d, 05.60.Gg

*Electronic address: gerasym@imath.kiev.ua

The aim of this work is to consider the links between consistent and approximate descriptions of the quantum-classical systems [1]-[7], i.e. systems are composed of two interacting subsystems, one of which behaves almost classically while the other requires a quantum description. The formulation of a quantum-classical dynamics has attracted considerable interests for the last decade [1], and as is well known, many conceptual difficulties arise in making this. It will be shown that mixed quantum-classical dynamics is described by the quantum-classical Heisenberg equation for the evolution of observables or by the quantum-classical Liouville equation for the evolution of states [1],[2],[4]-[6]. These systems can be described by the self-consistent Hamilton and Schrödinger equations set only as an uncorrelated approximation.

A description of quantum-classical systems is formulated in terms of two sets of objects: observables and states. The mean value (mathematical expectation) of observables defines a duality between observables and states and as a consequence there exist two approaches to the description of the evolution.

An observable $A(X,\hat{X})$ of a quantum-classical system is a function of canonical variables X characterizing classical degrees of freedom and non-commuting self-adjoint operators $\hat{X}$ satisfying canonical commutation relations [4],[6]. For instance, the Hamiltonian of a quantum-classical system has the structure

$$H(X,\hat{X}) = H_c(X)\hat{I} + H_q(\hat{X}) + H_{\mathrm{int}}(X,\hat{X}),$$

where $\hat{I}$ is a unit operator, $H_c, H_q, H_{\mathrm{int}}$ are correspondingly, the Hamiltonian of the classical, quantum degrees of freedom and their interaction. Further, as an example, we will consider a one-dimensional system consisting of two interacting classical and quantum particles (with unit masses). In this case

$$H_c(X) = \frac{1}{2}p^2, \;\; H_q(\hat{X}) = \frac{1}{2}\hat{p}^2, \;\; H_{\mathrm{int}}(X,\hat{X}) = \Phi(q,\hat{q}),$$

where p, q are canonical variables of a classical particle, $\hat{q}, \hat{p}$ are self-adjoint operators satisfying canonical commutation relations and the function Φ is an interaction potential.

The mean value of the observable $A(X,\hat{X})$ at time instant $t\in\mathbb{R}$ is defined by the positive continuous linear functional on the space of observables which can be defined in two different ways

$$\begin{aligned}\langle A\rangle(t) &= \int dX\,\mathrm{Tr}\,A(t,X,\hat{X})D(0,X,\hat{X}) = \\ &= \int dX\,\mathrm{Tr}\,A(0,X,\hat{X})D(t,X,\hat{X}),\end{aligned} \tag{1}$$

where $A(0,X,\hat{X})$ is an observable at the initial instant $t=0$, $D(0,X,\hat{X})$ is the density operator depending on classical canonical variables and $\int dX\,\mathrm{Tr}\,D(0,X,\hat{X})=1$.

The evolution of observables $A(t)=A(t,X,\hat{X})$ is described by the initial-value problem of the quantum-classical Heisenberg equation

$$\begin{aligned}&\frac{\partial}{\partial t}A(t)=\mathcal{L}A(t),\\ &A(t)|_{t=0}=A(0),\end{aligned} \tag{2}$$

where the generator $\mathcal{L}$ of this evolution equation depends on the quantization rule of a quantum subsystem. In the case of the Weyl quantization it has the form [4],[6]

$$\mathcal{L}A(t)=-\frac{i}{\hbar}\big[A(t),H\big]+\frac{1}{2}\big(\big\{A(t),H\big\}-\big\{H,A(t)\big\}\big), \tag{3}$$

where $H=H(X,\hat{X})$ is the Hamiltonian, $[\,.\,,.\,]$ is a commutator of operators and $\{\,.\,,.\,\}$ is the Poisson brackets. For some other quantization rules the operator $\mathcal{L}$ is defined in [4],[6].

In the case of a one-dimensional system consisting of two interacting classical and quantum particles in the configuration representation expression (3) has a form

$$\begin{aligned}\big(\mathcal{L}A\big)(q,p;\xi,\xi') = \quad & -\frac{i}{\hbar}\Big(-\frac{\hbar^2}{2}(-\Delta_\xi+\Delta_{\xi'})+\big(\Phi(\xi-q)-\Phi(\xi'-q)\big)\Big)\,A(q,p;\xi,\xi')+\\ &+\Big(p\frac{\partial}{\partial q}-\frac{\partial}{\partial q}\big(\Phi(\xi-q)-\Phi(\xi'-q)\big)\frac{\partial}{\partial p}\Big)\,A(q,p;\xi,\xi'),\end{aligned}$$

where $A(q,p;\xi,\xi')$ is a kernel of the operator $A(X,\hat{X})$ in the configuration representation, and in the Wigner representation it is as follow

$$\begin{aligned}\big(\mathcal{L}A\big)(x_1,x_2) \quad &= \sum_{j=1}^{2}p_j\frac{\partial}{\partial q_j}A(x_1,x_2)-\frac{\partial}{\partial q_1}\Phi(q_1-q_2)\frac{\partial}{\partial p_1}A(x_1,x_2)+\\ &+\frac{i}{2\pi\hbar}\int d\eta d\xi\,e^{i(p_2-\xi)\eta}\,\Big(\Phi\big(q_1-(q_2-\frac{\hbar}{2}\eta)\big)-\Phi\big(q_1-(q_2+\frac{\hbar}{2}\eta)\big)\Big)\,A(x_1,q_2,\xi),\end{aligned}$$

where $x_i\equiv(q_i,p_i)\in\mathbb{R}\times\mathbb{R}$ and $A(x_1,x_2)$ is a symbol of the operator $A(X,\hat{X})$.

Usually the evolution of a quantum-classical system is described, in the framework of evolution of states (the Schrödinger picture of evolution), by the initial-value problem dual to (2), namely, the quantum-classical Liouville equation [1],[4],[6]

$$\begin{aligned} &\frac{\partial}{\partial t}D(t) = -\mathcal{L}D(t), \\ &D(t)|_{t=0} = D(0). \end{aligned} \tag{4}$$

First, let us construct the self-consistent field approximation of this equation. For that we introduce the marginal states of classical and quantum subsystems correspondingly

$$D(t,X) = \mathrm{Tr}\, D(t,X,\hat{X}), \tag{5}$$

$$\hat{\rho}(t) = \int dX\, D(t,X,\hat{X}) \tag{6}$$

and the correlation operator of classical and quantum subsystems

$$g(t,X,\hat{X}) = D(t,X,\hat{X}) - D(t,X)\,\hat{\rho}(t). \tag{7}$$

If we assume that at any instant of time there are no correlations between classical and quantum particles, i.e. it holds $g(t,X,\hat{X}) = 0$, then in such an uncorrelated approximation we derive from (4) a self-consistent equations set of the Liouville and von Neumann equations for marginal states (5),(6) of classical and quantum subsystems

$$\frac{\partial}{\partial t}D(t,X) = \big\{H_c(X) + \mathrm{Tr}\, H_{\mathrm{int}}(X,\hat{X})\,\hat{\rho}(t)\,,\; D(t,X)\big\}, \tag{8}$$

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}(t) = \big[H_q(\hat{X}) + \int dX\, H_{\mathrm{int}}(X,\hat{X})\, D(t,X)\,,\; \hat{\rho}(t)\big] \tag{9}$$

with initial data

$$\begin{aligned} &D(t)|_{t=0} = D(0), \\ &\hat{\rho}(t)|_{t=0} = \hat{\rho}(0). \end{aligned}$$

We note that the initial-value problem of equations (8),(9) describes the evolution of all possible states of quantum-classical systems if correlations between classical and quantum particles are neglected (the self-consistent field approximation). This type of approximation can not be treated as the mean-field approximation since we consider finitely many particles while the mean-field approximation assumes the transition to the thermodynamic limit, i.e. it has a sense for infinitely many particles. Rigorous results about the mean-field limit of

dynamics of quantum many-particle systems in the framework of evolution of observables and states are given in [8].

Let at the initial instant the states of quantum and classical subsystems be pure states, i.e.

$$D(0,X)=\delta\big(X-X_0\big), \tag{10}$$
$$\hat{\rho}(0,\xi,\xi')=\Psi_0(\xi)\Psi_0^*(\xi'),$$

where $\delta(X-X_0)$ is a Dirac measure, X_0 is the phase space point in which we measure observables of classical subsystem, $\hat{\rho}(0,\xi,\xi')$ is a kernel (a density matrix) of marginal density operator (6) in the configuration representation, which is the projector operator on the vector $\Psi_0\in L^2$. We remark that the problem how to define a pure state of the whole quantum-classical system is an open problem.

Then in the configuration representation the initial-value problem of equations (8),(9) is an equivalent to the initial-value problem of a self-consistent set of the Hamilton and Schrödinger equations

$$\frac{\partial}{\partial t}X(t)=\big\{X(t)\,,\,H_c(X)+\int d\xi\,H_{\mathrm{int}}(X;\xi,\xi)\,|\Psi(t,\xi)|^2\big\}, \tag{11}$$
$$i\hbar\frac{\partial}{\partial t}\Psi(t,\xi)=\int d\xi'\big(H_q(\xi,\xi')+H_{\mathrm{int}}(X(t);\xi,\xi')\big)\Psi(t,\xi') \tag{12}$$

with initial data

$$X(t)|_{t=0}=X,$$
$$\Psi(t,\xi)|_{t=0}=\Psi_0(\xi).$$

For example, in the case of a one-dimensional system consisting of two interacting classical and quantum particles (with unit masses) equations (11),(12) get the form

$$\frac{d^2}{dt^2}Q(t)=-\frac{\partial}{\partial Q(t)}\int d\xi\,\Phi(Q(t)-\xi)\,|\Psi(t,\xi)|^2,$$
$$i\hbar\frac{\partial}{\partial t}\Psi(t,\xi)=-\frac{\hbar^2}{2}\frac{\partial^2}{\partial\xi^2}\Psi(t,\xi)+\Phi(Q(t)-\xi)\Psi(t,\xi)$$

with initial data ($X\equiv(q,v)$)

$$Q(t)|_{t=0}=q,\quad \frac{d}{dt}Q(t)|_{t=0}=v,$$
$$\Psi(t,\xi)|_{t=0}=\Psi_0(\xi),$$

where $\Phi(|Q(t)-\xi|)$ is a two-body interaction potential, $Q(t)$ is a position at the instant t of a classical particle in the space. Such a self-consistent set of the Newton and Schrödinger equations is usually used for the description of the evolution of states of quantum-classical systems.

Now we consider the description of a quantum-classical system in the uncorrelated approximation (7) between classical and quantum particles in the framework of evolution of observables (the Heisenberg picture of evolution).

Assume that a quantum-classical system is in an uncorrelated pure state (10), i.e.

$$D(0,X;\hat{X}) = \delta\big(X-X_0\big)P_{\Psi_0}, \tag{13}$$

where $P_{\Psi_0} \equiv (\Psi_0,\,.\,)\Psi_0$ (or in Dirac notation: $P_{\Psi_0} \equiv |\Psi_0\rangle\langle\Psi_0|$) is a one-dimensional projector onto a unit vector Ψ_0 from a Hilbert space. In the configuration representation a kernel of operator (13) has the form

$$D(0,X;\xi,\xi') = \delta\big(X-X_0\big)\Psi_0(\xi)\Psi_0^*(\xi').$$

Then according to (1) in this approximation the evolution of the canonical observables of quantum and classical particles is described by the Heisenberg equations set

$$\frac{\partial}{\partial t}X(t)\hat{I} = \big\{X(t)\hat{I}\,,\,H_c(X)\hat{I}+H_{\mathrm{int}}(X,\hat{X})\big\}, \tag{14}$$

$$i\hbar\frac{\partial}{\partial t}\hat{X}(t) = \big[\hat{X}(t)\,,\,H_q(\hat{X})+H_{\mathrm{int}}(X,\hat{X})\big] \tag{15}$$

with initial data

$$X(t)|_{t=0} = X,$$
$$\hat{X}(t)|_{t=0} = \hat{X}.$$

For example, in the case of a one-dimensional system consisting of two interacting classical and quantum particles equations (14),(15) can be rewritten for pairs of canonically conjugated variables $X(t)=\big(Q(t),P(t)\big)$ and $\hat{X}(t)=\big(\hat{Q}(t),\hat{P}(t)\big)$ in the following form

$$\frac{d}{dt}Q(t) = P(t),$$
$$\frac{d}{dt}P(t)\hat{I} = -\frac{\partial}{\partial Q(t)}\Phi(Q(t),\hat{Q}(t)),$$
$$\frac{d}{dt}\hat{Q}(t) = \hat{P}(t),$$
$$\frac{d}{dt}\hat{P}(t) = -\Phi'(Q(t),\hat{Q}(t)),$$

where the function Φ' is the derivative of the function Φ. These equations can also be rewritten similar to (11),(12) as equations in the configuration representation. In the Wigner representation they take the following fascinating form

$$\begin{aligned}
&\frac{d}{dt}Q_1(t) = P_1(t),\\
&\frac{d}{dt}P_1(t) = -\frac{\partial}{\partial Q_1(t)}\Phi(Q_1(t) - Q_2(t)),\\
&\frac{d}{dt}Q_2(t) = P_2(t),\\
&\frac{d}{dt}P_2(t) = -\frac{\partial}{\partial Q_2(t)}\Phi(Q_1(t) - Q_2(t))
\end{aligned}$$

with initial data

$$X_1(t)|_{t=0} = x_1, \;\; X_2(t)|_{t=0} = x_2,$$

where $X_i(t) \equiv \big(Q_i(t), P_i(t)\big)$, $i = 1, 2$, and $X_2(t) \equiv \big(Q_2(t), P_2(t)\big)$ are symbols of the operators $\hat{X}(t) = \big(\hat{Q}(t), \hat{P}(t)\big)$. We note that in this representation a symbol of uncorrelated pure state (13) defines by the following Wigner function

$$D(0, x_1, x_2) = (2\pi)^{-1}\delta\big(x_1 - x_0\big)\int d\xi\, \Psi_0\big(q_2 + \frac{1}{2}\hbar\,\xi\big)\Psi_0^*\big(q_2 - \frac{1}{2}\hbar\,\xi\big)e^{-i\xi p_2}$$

and mean value (1) of an observable is given by the following functional

$$\langle A\rangle(t) = (2\pi\hbar)^{-1}\int dx_1 dx_2\, A(t, x_1, x_2)\, D(0, x_1, x_2).$$

In summary, mixed quantum-classical dynamics is described by the quantum-classical Heisenberg equation (2) in the framework of the evolution of observables or by the quantum-classical Liouville equation (4) in the framework of the evolution of states. A quantum-classical system can be described by the self-consistent Hamilton (11) and Schrödinger (12) equations set or by the self-consistent Hamilton (14) and Heisenberg (15) equations set and state (13) only in an uncorrelated approximation [5],[6].

---

[1] R. Kapral, Annu. Rev. Phys. Chem. **57**, 1239 (2006).

[2] G. Ciccotti, D. Coker and R. Kapral, *Quantum Dynamics of Complex Molecular Systems*, Eds., D. A. Micha and I. Burghardt (Springer, 2007), p. 275.

[3] V.I. Gerasimenko and D.Ya. Petrina, Theor. Math. Phys. **42**, 88 (1980).

[4] V.I. Gerasimenko, Preprint 80–92P, Kiev: Inst. Theor. Phys. (1980).

[5] V.I. Gerasimenko, Reports of Acad. Sci. Ukrainian SSR. **10**, 65 (1981).

[6] V.I. Gerasimenko, Theor. Math. Phys. **50**, 77 (1982).

[7] V.I. Gerasimenko, V.Z. Enolski and D.Ya. Petrina, Doklady Akad. Nauk USSR, **315**, 75 (1990).

[8] V.I. Gerasimenko, arXiv:0908.2797v1 (2009).